ACETONITRILE

Acetonitrile is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 75-05-8 CH_3CN

Molecular Formula: C_2H_3N

Acetonitrile is a liquid at room temperature and has an ether-like odor. Acetonitrile is miscible with water, methanol, methyl acetate, acetone, ether, chloroform, carbon tetrachloride, and many saturated and unsaturated hydrocarbons. It is immiscible with many saturated hydrocarbons (petroleum fractions). Acetonitrile burns with a luminous flame (Merck, 1989).

Physical Properties of Acetonitrile

Synonyms: methyl cyanide; cyanomethane; ethanenitrile

Molecular Weight:	41.05
Boiling Point:	81.6 °C
Melting Point:	-45 °C
Flash Point:	12.8 °C (55 °F)
Vapor Pressure	74 mm Hg at 20 °C
Density/Specific Gravity:	0.78745 at 15/4 °C 0.7138 at 30/4 °C
Vapor Density:	1.42 (air = 1)
Log Octanol/Water Partition Coefficient:	-0.34
Henry's Law Constant:	2.93×10^{-5} atm-m^3/mole
Conversion Factor:	1 ppm = 1.68 mg/m^3

(Howard, 1990; Merck, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

Acetonitrile is used in organic synthesis, acrylic fibers, pharmaceuticals, perfumes, and in nitrile rubber. It is also used as a solvent and as a chemical intermediate. Acetonitrile is found in

automobile exhaust and cigarette smoke (Howard, 1990). Other sources of acetonitrile include: synthetic rubber manufacturing, acrylonitrile manufacturing, shale oil retorting, coal gasification, and incineration of polyacrylonitrile. Thermal decomposition products of flexible polyurethane foam are also a source of acetonitrile (HSDB, 1991). The primary stationary sources that have reported emissions of acetonitrile in California are miscellaneous chemical products manufacturing and coating, engraving, and allied services (ARB, 1997b).

B. Emissions

The total emissions of acetonitrile from stationary sources in California are estimated to be at least 810 pounds per year, based on data reported under the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

Acetonitrile occurs naturally in small amounts in coal tar (HSDB, 1991).

AMBIENT CONCENTRATIONS

No Air Resources Board data exist for ambient concentrations of acetonitrile. However, the United States Environmental Protection Agency (U.S. EPA) has compiled information from two United States cities that reported a maximum ambient concentration of 0.16 micrograms per cubic meter ($\mu g/m^3$) or 0.10 parts per billion (ppb) in 1982 with a mean ambient air concentration of 0.05 $\mu g/m^3$ or 0.03 ppb (U.S. EPA, 1993a).

INDOOR SOURCES AND CONCENTRATIONS

No information about the indoor sources and concentrations of acetonitrile was found in the readily-available literature.

ATMOSPHERIC PERSISTENCE

Acetonitrile exists in the atmosphere in the gas phase. The dominant tropospheric chemical removal process is by its gas phase reaction with the hydroxyl radical (OH). The calculated half-life of acetonitrile due to its gas phase reaction with the OH radical is estimated to be approximately 1.5 years (Atkinson, 1995). It will persist in the troposphere for a long time and may be transported long distances from its emission source. Wet deposition may remove some atmospheric acetonitrile (Howard, 1990).

AB 2588 RISK ASSESSMENT INFORMATION

Although acetonitrile is reported as being emitted in California from stationary sources, no health values (cancer or non-cancer) are listed in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program Revised 1992 Risk Assessment Guidelines for use in risk assessments (CAPCOA, 1993).

HEALTH EFFECTS

Probable routes of human exposure to acetonitrile are inhalation and dermal contact (U.S. EPA, 1994a).

Non-Cancer: Exposure to acetonitrile vapors may cause irritation of skin, eyes, nose and throat, vomiting, convulsions, and death (Sittig, 1991). Overexposure may produce cyanide poisoning following metabolism to cyanide (HSDB, 1991).

The U.S. EPA is currently reviewing the Reference Concentration (RfC) for acetonitrile. The U.S. EPA has calculated (by an alternate method) a provisional RfC of 0.05 milligrams per cubic meter. The U.S. EPA has established an oral Reference Dose of (RfD) 0.006 milligrams per kilogram per day for acetonitrile based on decreased red blood cell counts and hematocrit, and hepatic lesions in mice. The U.S. EPA estimates that consumption of this dose or less, over a lifetime, would not result in the occurrence of chronic, non-cancer effects (U.S. EPA, 1994a).

No studies were located regarding adverse reproductive or developmental effects from exposure to acetonitrile in humans. Studies in test animals appear to suggest adverse developmental effects that include decreased average fetal weight and increased malformed offspring (U.S. EPA, 1994a).

Cancer: The National Toxicology Program is currently conducting a two-year carcinogenesis inhalation study on acetonitrile using rats and mice (U.S. EPA, 1994a). The International Agency for Research on Cancer and the U.S. EPA have not classified acetonitrile with respect to potential carcinogenicity (IARC, 1987a; U.S. EPA, 1994a).